An Introduction to Statistical Mechanics and the Ising Model

- A branch of physics that deals with systems with a large number of interacting elements.

  classic examples: gases
  fluids
  magnets ...

- A direct application of Mechanics to each of its individual parts is impossible due to the extreme size of the system - $N \sim 10^{23}$!

  $\nearrow$ Newton's Eqs.
  Hamilton Eqs.

☆ - However, if one looks at the macroscopic properties of these systems, such as P & T, they are well behave quantities.

  $\Rightarrow$ microscopic propertities must "average" out to give predictable macroscopic behavior for the whole system.

- This "averaging" property of large systems give us the ability to describe the system statistically — "statistical Mechanics".

Levels of complication

"Microcanonical Ensembles" : isolated systems with no exchange of energy or particles with its environment (E is conserved here)

- The energy E of the system is fixed by the Hamiltonian function $H(\underset{\sim}{x})$

  where $\underset{\sim}{x}$ is a high dimensional vector that specifies the configuration (state) of the system.

☆ - For large systems, there might be a large number of degenerate states for a given value of E.

For the sake of simplicity, suppose that the volume V of the system is its only relevant external parameter. An isolated system of this kind consists then of a given number N of particles in a specified volume V, the constant energy of the system being known to lie in some range between E and $E + \delta E$. Probability statements are then made with reference to an ensemble which consists of many such systems, all consisting of this number N of particles in this volume V, and all with their energy lying in the range between E and $E + \delta E$. The fundamental statistical postulate asserts that in an equilibrium situation the system is equally likely to be found in any one of its accessible states. Thus, if the energy of a system in state r is denoted by E_r, the probability P_r of finding the system in state r is given by

$$P_r = \begin{cases} C & \text{if } E < E_r < E + \delta E \\ 0 & \text{otherwise} \end{cases} \tag{6·1·1}$$

where C is a constant. It can be determined by the normalization condition that $\Sigma P_r = 1$ when summed over all accessible states in the range between E and $E + \delta E$.

An ensemble representing an isolated system in equilibrium consists then of systems distributed in accordance with (6·1·1). It is sometimes called a "microcanonical" ensemble.

6·2 *System in contact with a heat reservoir*

We consider the case of a small system A in thermal interaction with a heat reservoir A'. This is the situation already discussed in Sec. 3·6 where $A \ll A'$, i.e., where A has many fewer degrees of freedom than A'. The system A may be any relatively small *macro*scopic system. (For example, it may be a bottle of wine immersed in a swimming pool, the pool acting as a heat reservoir.) Sometimes it may also be a distinguishable *micro*scopic system which can be clearly identified.* (For example, it may be an atom at some lattice site in a solid, the solid acting as a heat reservoir.) We ask the following question: Under conditions of equilibrium, what is the probability P_r of finding the system A in any *one* particular microstate r of energy E_r?

This question is immediately answered by the same reasoning as was used in Sec. 3·3. We again assume weak interaction between A and A' so that their energies are additive. The energy of A is, of course, not fixed. It is only the total energy of the combined system $A^{(0)} = A + A'$ which has a constant value in some range between $E^{(0)}$ and $E^{(0)} + \delta E$. The conservation of energy can then be written as

$$E_r + E' = E^{(0)} \tag{6·2·1}$$

where E' denotes the energy of the reservoir A'. When A has an energy E_r,

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* The qualifying remark is introduced because it may not always be possible to label

the reservoir A' must then have an energy near $E' = E^{(0)} - E_r$. Hence, if . is in the *one* definite state r, the number of states accessible to the combine system $A^{(0)}$ is just the number of states $\Omega'(E^{(0)} - E_r)$ accessible to A' whe its energy lies in a range δE near the value $E' = E^{(0)} - E_r$. But, accordin to the fundamental statistical postulate, the probability of occurrence in th ensemble of a situation where A is in state r is simply proportional to th number of states accessible to $A^{(0)}$ under these conditions. Hence

▶ $$P_r = C'\Omega'(E^{(0)} - E_r) \qquad (6·2·2$$

where C' is a constant of proportionality independent of r. As usual, it can b determined from the normalization condition for probabilities, i.e.,

$$\sum_r P_r = 1 \tag{6·2·3}$$

where the sum extends over all possible states of A irrespective of energy.

Up to now, our discussion has been completely general. Let us now make use of the fact that A is a very much smaller system than A'. Then $E_r \ll E^{(0)}$ and (6·2·2) can be approximated by expanding the slowly varying logarithm of $\Omega'(E')$ about the value $E' = E^{(0)}$. Thus

$$\ln \Omega'(E^{(0)} - E_r) = \ln \Omega'(E^{(0)}) - \left[\frac{\partial \ln \Omega'}{\partial E'}\right]_0 E_r \cdots \tag{6·2·4}$$

Since A' acts as a heat reservoir, $E_r \lll E^{(0)}$ and higher-order terms in the expansion can be neglected. The derivative

$$\left[\frac{\partial \ln \Omega'}{\partial E'}\right]_0 \equiv \beta \tag{6·2·5}$$

is evaluated at the fixed energy $E' = E^{(0)}$ and is thus a constant independent of the energy E_r of A. By (3·3·10) it is just the constant temperature parameter $\beta = (kT)^{-1}$ characterizing the *heat reservoir* A'. (Physically, this means that the reservoir A' is so large compared to A that its temperature remains unaffected by whatever small amount of energy it gives to A.) Hence (6·2·4) becomes

$$\ln \Omega'(E^{(0)} - E_r) = \ln \Omega'(E^{(0)}) - \beta E_r$$

or

$$\Omega'(E^{(0)} - E_r) = \Omega'(E^{(0)})\, e^{-\beta E_r} \tag{6·2·6}$$

Since $\Omega'(E^{(0)})$ is just a constant independent of r, (6·2·2) becomes then simply

▶ $$P_r = C\, e^{-\beta E_r} \tag{6·2·7}$$

where C is some constant of proportionality independent of r. Using the normalization condition (6·2·3), C is determined by the relation

$$C^{-1} = \sum e^{-\beta E}$$

"Canoical ensembles" : systems are in thermal contact with a heat reservior.

- heat reservior is assummed to be big so that $T_{\text{reservoir}}$ can be considered fixed

  But, energy E can be exchanged between the reservior and the system.

- At a given temperature T, the system typically has access to a large # of allowed states!

Statistical Description of states

① let define

$R(\underset{\sim}{x} \to \underset{\sim}{x}')\,dt$ to be the probability that the system starting in state $\underset{\sim}{x}$ and ending up in state $\underset{\sim}{x}'$ after dt.

$R(\underset{\sim}{x} \to \underset{\sim}{x}')$ is called the transition rate.

- $R(\underset{\sim}{x} \to \underset{\sim}{x}')$ is usually assumed to be time independent!

② Now, we can also define a set of weights $W_{\underset{\sim}{x}}(t)$ that gives the probability in finding the system at state $\underset{\sim}{x}$ at time t.

③ Then, the time evolution of the system can be describe by the "master equation":

$$\frac{dw_{\underset{\sim}{x}}}{dt} = \sum_{\underset{\sim}{x}'} \left[W_{\underset{\sim}{x}'}(t) R(\underset{\sim}{x}' \to \underset{\sim}{x}) - W_{\underset{\sim}{x}}(t) R(\underset{\sim}{x} \to \underset{\sim}{x}') \right]$$

- this is just a statement on the conservation of probability.

Since, $W_{\underset{\sim}{x}}(t)$ is a probability, it must also satisfy:

$$\sum_{\underset{\sim}{x}} W_{\underset{\sim}{x}}(t) = 1, \quad \text{for all time.}$$

★ These two equations formally define $W_{\underset{\sim}{x}}(t)$!

④ With $W_{\underset{\sim}{x}}(t)$ known, then all macroscopic properties can be estimated.

For example, $E(\underset{\sim}{x})$ is the energy for a given state, then

sum over all allowed states within the given constraints.

$$\langle E \rangle = \sum_{\underset{\sim}{x}} E(\underset{\sim}{x})\, W_{\underset{\sim}{x}}(t)$$

gives the expectation of the energy for the system.

Equilibrium

Consider the situation when the rates of going into & out of $\underset{\sim}{x}$ exactly cancel, then $\frac{dW_{\underset{\sim}{x}}(t)}{dt} = 0$ or $W_{\underset{\sim}{x}}(t)$ is constant in time.

- We would call the system to be in equilibrium.

☆ Since the master equation is of 1st order and $W_{\underset{\sim}{x}}(t) \in [0, 1]$ (probability), all systems governed by this equation must → equilibrium at large t.

☆☆ For systems in equilibrium, $R(\underset{\sim}{x} \to \underset{\sim}{x}')$ must take on specific values!

☆☆ For systems in equilibrium, we known how the equilibrium occupation probability

$$\rho(\underset{\sim}{x}) = \lim_{t \to \infty} W_{\underset{\sim}{x}}(t)$$

should behave. (Gibb 1902, Boltzman)

Boltzman's constant

$$\rightarrow \quad \rho(\underset{\sim}{x}) = \frac{1}{Z} e^{-E(\underset{\sim}{x})/KT}$$

$$\beta = \frac{1}{KT}$$

where $Z = \sum_{\underset{\sim}{x}} e^{-E(\underset{\sim}{x})/KT} = \sum_{\underset{\sim}{x}} e^{-\beta E(\underset{\sim}{x})}$

is called the partition function.

– Z is also the normalization factor.

– $\rho(\underset{\sim}{x})$ is called the Boltzman's Distribution

So, in terms of $P(\underset{\sim}{x})$, macroscopic averages are,

$$\langle Q \rangle = \sum_{\underset{\sim}{x}} P(\underset{\sim}{x})\, Q(\underset{\sim}{x}) = \frac{1}{Z} \sum_{\underset{\sim}{x}} Q(\underset{\sim}{x})\, e^{-\beta E(\underset{\sim}{x})}$$

In particular, the expectation value of the energy $\langle E \rangle$ (the internal energy of the system) is

$$U = \frac{1}{Z} \sum_{\underset{\sim}{x}} E(\underset{\sim}{x})\, e^{-\beta E(\underset{\sim}{x})}$$

Note. This can also be written in terms of Z,

$$U = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = -\frac{\partial \log Z}{\partial \beta}$$

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check:

$$\frac{\partial Z}{\partial \beta} = \frac{\partial}{\partial \beta}\left(\sum_{\underset{\sim}{x}} e^{-\beta E(\underset{\sim}{x})}\right)$$

$$= \sum_{\underset{\sim}{x}} \left(-E(\underset{\sim}{x})\, e^{-\beta E(\underset{\sim}{x})}\right)$$

$$-\frac{1}{Z}\frac{\partial Z}{\partial \beta} = \frac{1}{Z} \sum_{\underset{\sim}{x}} E(\underset{\sim}{x})\, e^{-\beta E(\underset{\sim}{x})}$$

And, specific heat is,

$dT = -\frac{1}{k\beta^2}\,d\beta$ $\qquad$ $U = -\frac{\partial \log Z}{\partial \beta}$

$$C \equiv \frac{\partial U}{\partial T} = -k\beta^2 \frac{\partial U}{\partial \beta} = k\beta^2 \frac{\partial^2 \log Z}{\partial \beta^2}$$

recall $\beta = \frac{1}{kT}$

Then, from thermodynamic relations, we have

$$C = T\frac{\partial S}{\partial T} = -\beta \frac{\partial S}{\partial \beta}$$

So,

$$S = \int -\frac{C}{\beta}\,d\beta$$

$$= -\int k\beta \frac{\partial^2 \log Z}{\partial \beta^2}\,d\beta$$

$u = k\beta$ $\qquad$ $dv = \frac{\partial^2 \log Z}{\partial \beta^2}\,d\beta$

$du = k\,d\beta$ $\qquad$ $v = \frac{\partial \log Z}{\partial \beta}$

$$= -k\beta \frac{\partial \log Z}{\partial \beta} + \int \frac{\partial \log Z}{\partial \beta}\,k\,d\beta$$

$$\underline{S = -k\beta \frac{\partial \log Z}{\partial \beta} + k \log Z}$$

Then, the free energy is given by

$$F = U - TS = -\cancel{\frac{\partial \log Z}{\partial \beta}} - \overset{T}{\frac{1}{k\beta}}\left(-\cancel{k\beta\frac{\partial \log Z}{\partial \beta}} + k\log Z\right)$$

$$= -kT\log Z$$

Then, with F, we can calculate all the "conjugate" forces to the system:

$$P = -\frac{\partial F}{\partial V} \qquad M = \frac{\partial F}{\partial B}$$

$$(P, V) \qquad (M, B)$$

☆ Z (the partition function) is an important quantity in statistical physics.

In numerical simulations, it is important to be able calculate Z efficiently!

- All macroscopic thermodynamic quantities can be derived by taking the appropriate derivatives of Z with respect to β, V, B, etc. –

Calculating C more directly :

- Consider the variance of E :

$$\begin{aligned}
&\langle (E - \langle E\rangle)^2 \rangle \\
&= \langle E^2 - 2E\langle E\rangle + \langle E\rangle^2 \rangle \\
&= \langle E^2\rangle - 2\langle E\rangle^2 + \langle E\rangle^2 \\
&= \langle E^2\rangle - \langle E\rangle^2
\end{aligned}$$

Now, $\langle E^2\rangle = \frac{1}{Z}\sum_{\underset{\sim}{x}} E^2(\underset{\sim}{x})\, e^{-\beta E(\underset{\sim}{x})}$

$$= \frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2}$$

$$\langle E\rangle^2 = \left(\frac{1}{Z}\frac{\partial Z}{\partial \beta}\right)^2$$

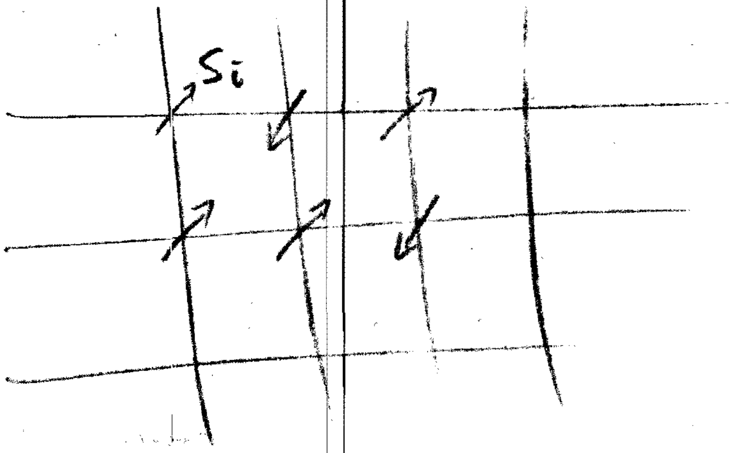
Note: $\frac{\partial}{\partial\beta}\left(\frac{\partial \log Z}{\partial \beta}\right) = \frac{\partial}{\partial\beta}\left(\frac{1}{Z}\frac{\partial Z}{\partial\beta}\right)$

$$\underset{\underset{\displaystyle \frac{C}{k\beta^2}}{\uparrow}}{\phantom{\frac{\partial}{\partial\beta}}} \quad = \underset{\underset{\displaystyle \langle E^2\rangle}{\uparrow}}{\frac{1}{Z}\frac{\partial^2 Z}{\partial\beta^2}} - \underset{\displaystyle \langle E\rangle^2}{\frac{1}{Z^2}\frac{\partial Z}{\partial\beta}\frac{\partial Z}{\partial\beta}}$$

The Ising Model

- A simple model for a magnet.

Model



- Macroscopic magneticism is resulted from a collection of magnetic dipoles or atomic spins S_i.

- The spins are assumed to be on a fixed lattice $\left(\begin{array}{ll} \text{3D} & \text{physical} \\ \text{2D} & \text{simplified system chosen} \end{array} \right)$

Note: 1D & 2D can be solved analytically (Onsager 1944)
3D is still unresolved analytically.

- S_i can be up (+1) or down (−1)

  (other types exist such as
  Continuous spin models : XY 2D
  Heisenberg 3D)

- interactions are of the nearest neighbor type.

☆ → this model provides a picture on how the system phase transition from a paramagnetic state to a ferromagnetic state as

$T < T_c$!

$$\begin{cases} \text{paramagnetic} \longrightarrow \overset{\text{mean}}{\text{Magnetization}} = 0 \\ \text{ferromagnetic} \longrightarrow \langle M \rangle \neq 0 . \end{cases} \Big\} \text{ in zero field}$$

The system is characterized by the Hamiltonian

$$H = -J \overset{\text{int with each others}}{\sum_{\langle ij \rangle} S_i S_j} - B \overset{\text{int with external B field}}{\sum_j S_j}$$

↑ summing over NN

↖ For this simulation, take B = 0.

Then, the partition function is given by

$$Z = \sum_{\{s_i\}} e^{-\beta H}$$

$\uparrow$

summing all possible combination of $\{s_i\}$

with a given energy $E \,(= H)$.

- $\langle M \rangle = \left\langle \sum_i s_i \right\rangle_{\text{over encemble}}$

  mean magnetization

  $\uparrow$ over all spins on one grid

- $\langle m \rangle = \dfrac{\langle M \rangle}{N}$

  mean magnetization per spin

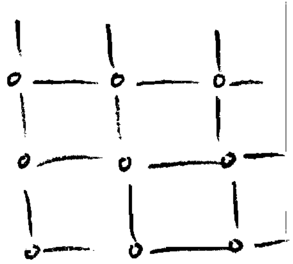
Counting Bonds on Ising Grid

$H = -J \sum_{\langle ij \rangle} S_i S_j$ — sum over all bonds

with periodic boundary

For N×N grid, $\underline{H = -2N^2}$ for all up or down arrangement.

- $\underline{N=3}$:



3×3 vertical bonds

3×3 horizontal bonds

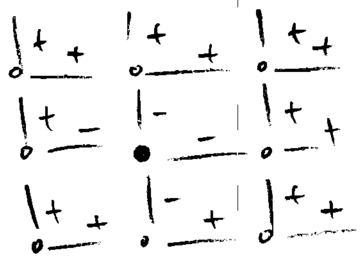
$2 \times 3 \times 3$ total bonds

$H = -18$

- With one spin flip at middle

$$E_{x'} = E_x + 2J S^x_{ij} \sum_{nn} S^x_{ij}$$

$$= -18 + 8 = -10$$



6 actual count = 10

0

4

$E_x' = -10$